Quantum theory of shuttling instability in a movable quantum dot array

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Abstract. We study the shuttling instability in an array of three quantum dots the central one of which is movable. We extend the results by Armour and MacKinnon on this problem to a broader parameter regime. The results obtained by an efficient numerical method are interpreted directly using the Wigner distributions. We emphasize that the instability should be viewed as a crossover phenomenon rather than a clear-cut transition.

1. Introduction

Since the first proposal by Gorelik et al. [1] of the shuttling instability in a generic nanoelectromechanical system (NEMS) consisting in a movable single electron transistor the phenomenon of the shuttling transport attracted much attention. However, until recently the fully quantum theory of the phenomenon was not developed. The first quantum mechanical study on a modified setup was accomplished by Armour and MacKinnon [2], closely followed by the work of the present authors on the original Gorelik's setup [3]. In this paper we extend the results by Armour and MacKinnon. The phase space analysis in terms of the Wigner functions introduced in [3] reveals directly the nature of the transport (incoherent tunnelling versus shuttling) in different regions in contrast to the indirect evidence used by Armour and MacKinnon. Also the new numerical scheme that we use enables us to access a wider range of parameters fast and reliably.

2. Model and method of solution

Let us consider a simple NEMS consisting of an array of three quantum dots (device) connected to two leads [2]. The central dot is assumed to be movable in a parabolic potential. The Hamiltonian of the device consists of the mechanical and the electronic parts $H = H_{\rm mech} + H_{\rm el}$ where $H_{\rm mech} = \hbar\omega\hat{a}^\dagger\hat{a}$ is the Hamiltonian of the harmonic oscillator and $H_{\rm el} = \sum_{\alpha,\beta\in\{0,L,C,R\}} |\alpha\rangle\epsilon_{\alpha\beta}(\hat{x})\langle\beta|$. We assume strong Coulomb blockade regime with no double occupancies so that the vectors $|\alpha\rangle$ with

$\alpha = 0, L, C, R$ span the entire electronic Hilbert space of the device. Each matrix element $\epsilon_{\alpha\beta}(\hat{x})$ is still a full matrix in the oscillator space. $\epsilon(\hat{x})$ reads explicitly

$$\epsilon(\hat{x}) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{\Delta V}{2} & t_L(\hat{x}) & 0 \\ 0 & t_L(\hat{x}) & -\frac{\Delta V}{2x_0}\hat{x} & t_R(\hat{x}) \\ 0 & 0 & t_R(\hat{x}) & -\frac{\Delta V}{2} \end{bmatrix} \tag{1}$$

where $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^\dagger)$ is the position operator, ΔV, the *device bias*, is the difference between the energy of the left and the right dot. x_0 is half the distance between the two outer dots and represents the maximum amplitude of the inner dot oscillation. The three dots are electrically connected only via a tunnelling mechanism. The tunnelling length is given by $1/\alpha$ and the tunnelling strengths depend on the position operator $\hat{x}$ of the inner grain as $t_L(\hat{x}) = V_0 e^{-\alpha(x_0+\hat{x})}$, $t_R(\hat{x}) = V_0 e^{-\alpha(x_0-\hat{x})}$.

The dynamics of the device is described by the generalized master equation (GME) formalism [2]. The density matrix of the device evolves according to $\dot{\rho} = -i[H,\rho] + \Xi\rho + \dot{\rho}_d$. The first term represents the coherent evolution of the isolated device. The coupling to the leads responsible for the electronic transfer from/to the device is introduced in the wide band approximation following Gurvitz et al. [4] and yields the second term in the equation (in the block notation of [2])

$$\Xi\rho = \Gamma \begin{bmatrix} \rho_{RR} - \rho_{00} & 0 & 0 & 0 \\ 0 & \rho_{00} & 0 & -\rho_{LR}/2 \\ 0 & 0 & 0 & -\rho_{CR}/2 \\ 0 & -\rho_{RL}/2 & -\rho_{RC}/2 & -\rho_{RR} \end{bmatrix} \tag{2}$$

with Γ being the injection rate to the leads. The third term describes the effect of the environment on the oscillator, consisting in mechanical damping and random quantum and thermal excitation (Langevin force). It reads [2]

$$\dot{\rho}_d = -\frac{\gamma}{2}\bar{n}(aa^\dagger\rho - 2a^\dagger\rho a + \rho aa^\dagger) - \frac{\gamma}{2}(\bar{n}+1)(a^\dagger a\rho - 2a\rho a^\dagger + \rho a^\dagger a) \tag{3}$$

where γ is the damping rate and $\bar{n}$ is the mean occupation number of the oscillator at temperature T.

The stationary version of the above GME was solved numerically after the oscillator Hilbert space was truncated at sufficiently large N so that all dynamically excited states were contained within the basis. Utilizing the decoupling properties of the GME in the block notation resulted in the problem of finding a unique null space of a (super)matrix with the linear dimension $10N^2$ (with up to $N = 40$). The Arnoldi iteration [5] with preconditioning was found to be superior to direct methods, such as singular value decomposition or inverse iteration. The preconditioning involving the inversion of the Sylvester part of the problem (a fast procedure) is crucial for the convergence of the method which is very fast and low memory consuming (the whole (super)matrix does not have to be stored in the memory).

3. Results and discussion

The resulting stationary density matrix was used to evaluate the mean value of current $I = \Gamma \,\mathrm{Tr}_{\mathrm{osc}}\rho_{RR}$ [2] and the phase space distribution of the charged central dot using the transformation into Wigner coordinates [3]. These quantities as a function of the device bias ΔV and for three different values of the injection rate Γ are plotted

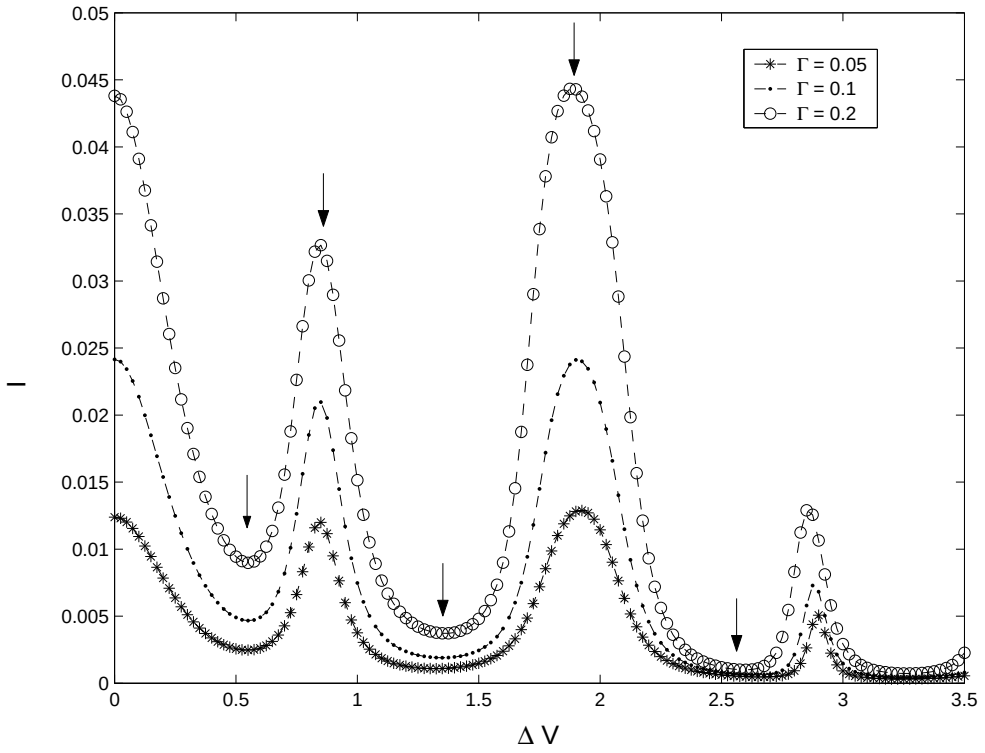

Figure 1. Plot of the current through the triple dot system as a function of the device bias for different injection rates Γ. The other parameters are $V_0 = 0.5$, $\alpha = 0.2$, $x_0 = 5$, $\gamma = 0.0125$, $\omega = 1$.

in the figures 1 and 2, respectively. It was found in [2] that the triple dot system exhibits different regimes of transport at different device biases. The current peaks at $\Delta V \approx n\omega$ (see figure 1) were identified as effects of electromechanical resonances within the device. Yet, the different peaks may correspond to different physical mechanisms — while the peak around $\Delta V \approx \omega$ is mainly due to the incoherent oscillator-assisted tunnelling the peak at $\Delta V \approx 2\omega$ reveals a clear shuttling component. This finding by Armour and MacKinnon based on indirect evidence of parametric dependencies of the current curves (e.g. the dependence of the current curve on the tunneling length $1/\alpha$) is confirmed by the direct inspection of the phase space distributions (see the first row of figure 2). The half-moon-like shape characteristic for shuttling transport [3] is only present around $\Delta V \approx 2\omega$ while all other plots show just the fuzzy spot indicative of incoherent tunnelling. However, our direct criterion for detecting the shuttling regime reveals a close similarity between the resonances. For increasing injection rate we can see that the shuttling regime gradually sets in also in the vicinity of the first resonance peak. This reveals the crossover character of the onset of the shuttling instability found also previously [3]. The sharp transition into the shuttling regime reported in semiclassical studies is smeared into the crossover due to the noise present in the system and properly accounted for in our approach.

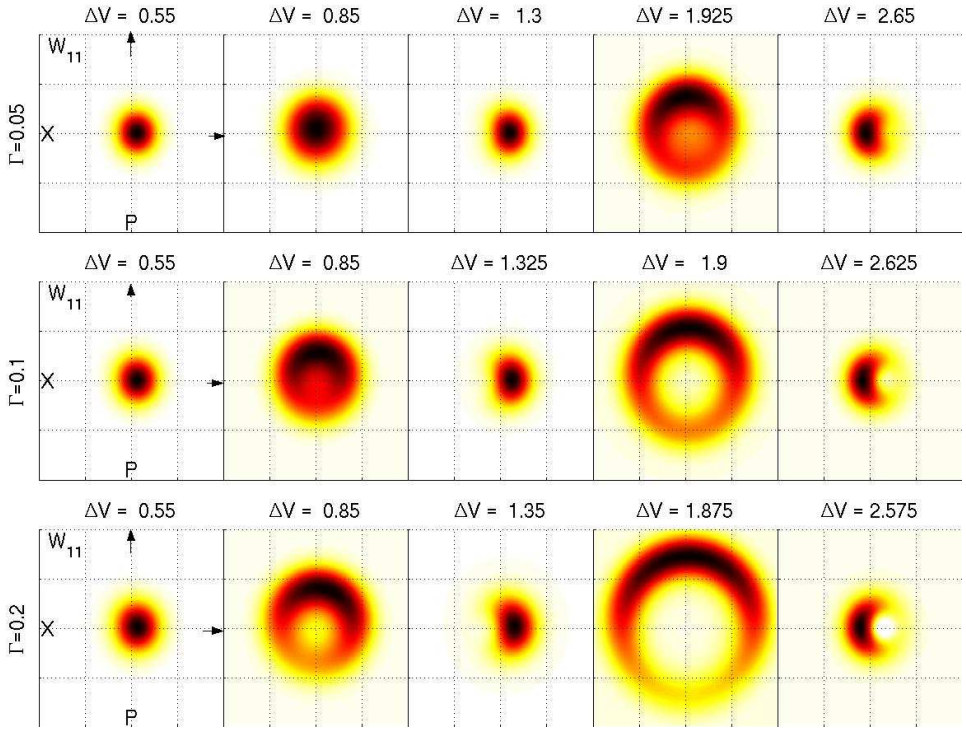

Figure 2. Wigner distributions for the central dot in the charged state. Different device biases are the points of minimum or maximum current (see figure 1).

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